Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-

Other names:	Acetophenone, 4'-hydroxy-3',5'-dimethoxy- Acetosyringone 1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone 4'-Hydroxy-3',5'-dimethoxyacetophenone 3',5'-Dimethoxy-4'-hydroxyacetophenone Acetosyringon 3,5-Dimethoxy-4-hydroxyacetophenone Acetophenone, 3,5-dimethoxy-4-hydroxy- 4-Hydroksy-3',5'-dwumetoksyacetofenon 4-Acetylsyringol Phenol, 4-acetyl-2,6-dimethoxy 1-(4-Hydroxy-3,5-dimethoxyphenyl)-ethanone (acetosyringone)
Inchi:	InChI=1S/C10H12O4/c1-6(11)7-4-8(13-2)10(12)9(5-7)14-3/h4-5,12H,1-3H3
InchiKey:	OJOBTAOGJIWAGB-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COc1cc(C(C)=O)cc(OC)c1O
Mol. weight [g/mol]:	196.20
CAS:	2478-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-367.07	kJ/mol	Joback Method
hf	-590.47	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.612		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1740.70		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1744.00		NIST Webbook
tb	644.17	K	Joback Method
tc	866.56	K	Joback Method
tf	460.03	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.54	J/mol×K	644.17	Joback Method
cpg	423.15	J/mol×K	829.49	Joback Method
cpg	413.99	J/mol×K	792.43	Joback Method
cpg	404.28	J/mol×K	755.36	Joback Method
cpg	393.99	J/mol×K	718.30	Joback Method
cpg	383.08	J/mol×K	681.23	Joback Method
cpg	431.80	J/mol×K	866.56	Joback Method
dvisc	0.0000209	Pa×s	644.17	Joback Method
dvisc	0.0000290	Pa×s	613.48	Joback Method
dvisc	0.0000415	Pa×s	582.79	Joback Method
dvisc	0.0000619	Pa×s	552.10	Joback Method
dvisc	0.0000967	Pa×s	521.41	Joback Method
dvisc	0.0001598	Pa×s	490.72	Joback Method
dvisc	0.0002824	Pa×s	460.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2478388&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume